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Solution of the Time-Dependent Schroedinger Equation using a Real Space Product Finite Element Discrete Variable Representation (RSPFEDVR) BARRY SCHNEIDER, National Science Foundation, LEE COLLINS, SUXING HU, Los Alamos National Laboratory — A novel approach to the solution of the time-dependent Schroedinger equation using a RSPFEDVR method is described. The method is applied in both a second and fourth order version. In this talk we describe the essential features of the approach and compare the method as to its accuracy and efficiency in a number of model problems. The method may be transparently and efficiently parallelized using MPI as a consequence of the structure of the RSPFEDVR propagator which leads to a minimal number of communications at each step in the propagation.

Prefer Oral Session
 Prefer Poster Session

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